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SOME IMPLICIT FINITE DIFFERENCE SCHEMES FOR HYPERBOLIC SYSTEMS

by

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ABSTRACT

Implicit finite difference schemes usually allow the use of large time steps. This could be an advantage in computing slowly varying solutions to hyperbolic systems. The usual Crank-Nicholson scheme as applied to a hyperbolic system is rather slow. This paper describes two modifications of the Crank-Nicholson scheme for hyperbolic systems which are implicit only in that they require the inversion of tridiagonal matrices. However, these schemes are unconditionally stable only for positive definite systems (supersonic flow). The results of computations using these schemes are described.

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SOME IMPLICIT FINITE DIFFERENCE SCHEMES FOR HYPERBOLIC SYSTEMS

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1. Introduction

In Section 2 we will describe the application of the Crank-Nicholson scheme to hyperbolic systems of equations. This method requires the inversion of a block-tridiagonal matrix. In order to speed up the computation we modify the scheme so that we need only invert scaler tridiagonal matrices. All of our results are for problems in one space dimension. These methods can be generalized to two dimensions but we have no analysis to indicate that the generalizations will work. In Section 3 we describe the numerical experiments used to check the accuracy and stability of these schemes. The equations of inviscid hydrodynamic flow were used in these calculations. In Section 4 we analyze the stability of these schemes using the method of von Neumann. In some cases we are unable to explicitly determine the eigenvalues of the amplification matrix so we are forced to compute the eigenvalues numerically.

2. Description of the Finite Difference Schemes

In this section we will describe some finite difference schemes of an implicit nature. For purposes of comparison we will begin with the usual Crank-Nicholson scheme [4]. This scheme is adapted to the nonlinear problem by use of a "predictor-corrector" method. We denote the hyperbolic system of equations by $\partial w/\partial t + A(w)\,\partial w/\partial x = 0$ where $A(w)$ is a matrix with real, distinct eigenvalues. If the equations are those of hydrodynamic flow we have

(2.1) $$A(w) = \begin{bmatrix} u & 0 & \rho \\ 0 & u & \gamma p \\ 0 & 1/\rho & u \end{bmatrix}, \qquad w = \begin{bmatrix} \rho \\ p \\ u \end{bmatrix},$$

where ρ, p, and u denote density, pressure and velocity and γ is the ratio of specific heats. We will use a mesh of equally spaced points (x_j, t_n) where $x_{j+1} - x_j = \Delta x$, $t_{n+1} - t_n = \Delta t$ and $1 \leq j \leq M$. We use the notation $w_j^n = w(x_j, t_n)$,

$$w_x = \frac{w(x+\Delta x, t) - w(x, t)}{\Delta x},$$

$$w_{\overline{x}} = \frac{w(x, t) - w(x-\Delta x, t)}{\Delta x},$$

$$w_{\hat{x}} = \frac{w(x+\Delta x, t) - w(x-\Delta x, t)}{2\,\Delta x}.$$

We shall assume the boundary values $w(x_1, t)$ and $w(x_M, t)$ are known and constant. Of course, this problem is not properly posed, but where the boundary conditions are known and constant this does not seem to cause any trouble

The first step in the Crank-Nicholson method is to predict the values of w_j^{n+1} by the use of an explicit difference scheme. We denote the predicted values by $w^{\#}$, and define them by

$$w^{\#} = w^n - \Delta t\, A(w^n)\, w_{\hat{x}}^n .$$

Then w^{n+1} is defined by the boundary conditions and the following equations

$$w^{n+1} = w^n - \frac{\Delta t}{2} A\left(\frac{w^n + w^{\#}}{2}\right)\left(w_{\hat{x}}^{n+1} + w_{\hat{x}}^n\right) .$$

The truncation error is $O(\Delta x^2 + \Delta t^2)$.

To solve these equations we use a method given by S. Schechter [5]. We may write the system as

$$\beta A_j w_{j+1}^{n+1} + w_j^{n+1} - \beta A_j w_{j-1}^{n+1} = D_j \quad ,$$

where $\beta = \Delta t/(4\Delta x)$, $A_j = A((w_j^{n+1} + w_j^{\#})/2)$ and D is a vector defined by

$$D_j = w_j^n - \beta A_j(w_{j+1}^n - w_{j-1}^n) \quad .$$

Thus the matrix of this system is block tridiagonal. The method is analogous to that used for a scaler tridiagonal system. We define matrices F_j and vectors G_j by recursion as follows: $F_1 = I$, $G_1 = D_1$, $F_j = I + \beta^2 A_j F_{j-1}^{-1} A_{j-1}$, and $G_j = D_j + \beta A_j F_{j-1}^{-1} D_{j-1}$. Then the solution is obtained by "backward substitution" $w_M^{n+1} = F_M^{-1} G_M$, $w_j^{n+1} = F_j^{-1}(G_j - \beta A_j w_{j+1}^{n+1})$.

To use this method we must be certain that the matrices F_j can be inverted without difficulty. If the matrix $A(w)$ is constant, then A has a complete set of distinct eigenvectors. These are also a complete set for the matrices F_j. If α is an eigenvalue of A_j and λ_j is the corresponding eigenvalue of F_j, then $1 + \beta^2\alpha^2/\lambda_j$ is the corresponding eigenvalue of F_{j+1}. Therefore $1 \leq \|F_j\| \leq 1 + a^2$ for $1 \leq j \leq M$, where $a \geq \beta\|A\|$. If the matrices A are all symmetric, then the norm of F_j satisfies the same inequality. In our case the matrices A_j are determined by equations (2.1) and are therefore neither symmetric nor constant. However, we had no difficulty in inverting the matrices F_j. An analysis by the method of von Neumann [4] shows this scheme to be unconditionally stable and this conclusion is supported by numerical experiments described in the following section.

We will next define a quasi-Crank-Nicholson (Q-C-N) scheme which is not centered in time. We define the lower triangular matrix A_L to consist of those elements of A on and below the diagonal with zero elements above the diagonal. We define A_U by $A_U = A - A_L$. Then the (Q-C-N) difference scheme is defined by

$$w^{n+1} = w^n - \Delta t\, A_L(w^n) w_{\hat{x}}^{n+1} - \Delta t\, A_U(w^n)\, w_{\hat{x}}^n \quad . \qquad (2.2)$$

To solve for each dependent variable we need only solve a system of equations

whose matrix is tridiagonal. Thus the scheme is effectively explicit. This is the reason for splitting the matrix into triangular parts. If the matrix $A(w)$ is defined by equations (2.1), then this scheme is unconditionally stable for supersonic flow and unconditionally unstable for subsonic flow. This will be discussed in Section 4. The truncation error is $O(\Delta t + \Delta x^2)$.

We can also define a quasi-Crank-Nicholson scheme which is centered in time. The first step is to predict the values of w^{n+1} by the equations

$$(2.3) \qquad w^{\#} = w^n - \Delta t\, A(w^n)\, w^n_{\hat{x}} \quad .$$

The centered Q-C-N scheme is then defined by the equations

$$(2.4) \qquad w^{n+1} = w^n - \frac{\Delta t}{2} A^{\#}_L w^{n+1}_{\hat{x}} - \frac{\Delta t}{2} A^{\#}_U w^{\#}_{\hat{x}} - \frac{\Delta t}{2} A^{\#} w^n_{\hat{x}} \quad ,$$

where $A^{\#} = A((w^n + w^{\#})/2)$. The solution of this system is obtained by solving a tridiagonal matrix equation for each dependent variable. The truncation error is $O(\Delta t^2 + \Delta x^2)$. In Section 4 we will show that this scheme is unconditionally stable for supersonic flow and conditionally stable for subsonic flow, provided that the matrix A is given by equations (2.1).

This centered quasi-Crank-Nicholson scheme was applied to the Navier-Stokes equations:

$$\frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial u}{\partial x} = 0 \quad ,$$

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + (\gamma - 1) T \frac{\partial u}{\partial x} = \frac{\gamma}{P_r R \rho} \frac{\partial^2 T}{\partial x^2} + \frac{4\gamma}{3\rho R} (\gamma - 1) \left(\frac{\partial u}{\partial x}\right)^2 \quad ,$$

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{1}{\gamma} \frac{\partial T}{\partial x} + \frac{T}{\gamma \rho} \frac{\partial \rho}{\partial x} = \frac{4}{3\rho R} \frac{\partial^2 u}{\partial x^2} \quad .$$

In these equations R represents the Reynolds number and P_r the Prandtl number. If these equations are differenced by the Lax-Wendroff method, then the stability condition is approximately

$$\Delta t < \min \left[\frac{\Delta x}{|u|+c}, \frac{3R\rho\, \Delta x^2}{16} \right] \quad [3].$$

There is a parabolic dependence on Δx. We have not determined a stability criterion for the centered Q-C-N method applied to the Navier-Stokes equations. However, enough computations were carried out to show that the stability condition depends on Δx^2 very weakly, if at all. Thus the stability condition is less stringent, especially for values of R which are not large.

It might be possible to use these methods for problems in two space dimensions by using alternating direction techniques. For example, suppose we wish to solve the system

$$\frac{\partial w}{\partial t} + A(w) \frac{\partial w}{\partial x} + B(w) \frac{\partial w}{\partial y} = 0 \quad .$$

The finite difference scheme could be

$$w^{\#} = w^n - \Delta t\, A_L^o\, w_{\hat{x}}^{\#} - \Delta t\, A_U^o\, w_{\hat{x}}^n - \Delta t\, B^o\, w_{\hat{y}}^n \quad ,$$

$$w^{n+1} = w^n - \Delta t\, A^1\, w_{\hat{x}}^{\#} - \Delta t\, B_L^1\, w_{\hat{y}}^{n+1} - \Delta t\, B_u^1\, w_{\hat{y}}^{\#} \quad ,$$

where $A^o = A(w^n)$ and $A^1 = A(1/2(w^{\#} + w^n))$. If this scheme is stable at all, it would probably be stable only for supersonic flow. The fact that the truncation error is first order in Δt may not be a major defect, particularly if the method is used to solve for a steady state solution. Perhaps it is possible to devise a scheme which is unconditionally stable for both subsonic and supersonic flow which involves nothing worse than the solution of scaler tridiagonal matrices.

3. Results of Numerical Computations

To test these schemes we used a hydrodynamic flow containing a simple rarefaction or compression wave. We applied the difference schemes to equations (2.1). The initial value $u(x, 0)$ was chosen to be constant in the neighborhoods of

x_1 and x_M (the boundary points) and monotone in between. The initial values $\rho(x, 0)$ and $p(x, 0)$ were computed from the equations below. This produces a simple wave moving on the characteristic with slope $u + c$.

$$\rho(x, 0) = \rho_o[1 + \frac{\gamma - 1}{2} \frac{u}{c_o}]^{2/(\gamma-1)} ,$$

$$p(x, 0) = \frac{p_o}{\rho_o} \rho(x, 0)^\gamma .$$

In these equations ρ_o, p_o, c_o represent the constant state ahead of the wave. The exact solution to this problem is easily calculated [1].

The results of the computation are shown in Table I. The number of points in the first column refers to the number of mesh points used to cover the interval over which $u(x, 0)$ is not constant. This determines the value of Δx. The value of Δt is given by $\Delta t = 0.9 \Delta x/(|u| + c)$ which is the Courant-Friedrichs-Lewy condition for stability. The uncentered Crank-Nicholson (C-N) scheme refers to one in which the coefficient matrix is not centered, that is:

$$w^{n+1} = w^n - \frac{\Delta t A(w^n)(w_{\hat{x}}^{n+1} + w_{\hat{x}}^n)}{2} .$$

In one case the quasi-Crank-Nicholson scheme was run with an initial value $u(x, 0)$ which had a continuous third derivative. In the other cases $u(x, 0) \in C^2$ but $\partial^3 u/\partial x^3$ was discontinuous at the head and tail of the rarefaction wave. If the truncation error is $O(\Delta x^2)$, the percentage error should drop by a factor of eight when the mesh spacing is halved. The percentage error given in the table is the maximum percentage error in the variables ρ, p, u throughout the mesh at 100 time steps. If the truncation error is to be $O(\Delta x^2)$, we must have $u \in C^3$. The flow is a simple rarefaction wave with Mach number $M_o = 2$ ahead of the wave and $M_1 = 1.75$ behind the wave. Other runs were made with $M_o = 0$ and $M_1 = 0.7$. In this case the error was about half that shown in the table. The computing time shown at the bottom of the table is the time required

Table I. Percentage error after 100 time steps for the various difference schemes.

No. of Points	C-N (A cen.)	C-N (A not cen.)	Q-C-N (cen.)	Q-C-N (cen.) $u \in C^3$	Q-C-N (not cen.)	Lax-Wend.
10	4.4%	4.7%	4.1%	4.8%	8.8%	2.0%
20	1.7	1.9	1.6	1.8	5.2	0.71
100	0.055	0.11	0.047	0.039	0.57	0.014
200	0.0087	0.042	0.0073	0.0050	0.15	0.0020
Computation time in milli-seconds per mesh point.	15	13	4.4	4.4	1.7	3.8

(in milli-seconds) to compute the solution at a single mesh point. Results of computing with the Lax-Wendroff scheme are shown for comparison. The equations used in the Lax-Wendroff scheme are written in conservation form. This accounts for much of the increase in accuracy. In Table I, C-N denotes Crank-Nicholson, Q-C-N quasi-Crank-Nicholson and cen. denotes a centered scheme.

4. Derivation of Stability Conditions

We will first derive a stability condition for the centered quasi-Crank-Nicholson scheme with the matrix $A(w)$ given by equations (2.1). We use the method of von Neumann, that is, we linearize the equations and assume a perturbation of the form $w^n = w(x_j, t_n) = k^n \exp(i\omega x_j)$. Substituting this value for w_j^n into equations (2.3) and (2.4) we obtain

$$
\begin{aligned}
k^{n+1} &= \left\{ I - \left[I + \frac{i\beta}{2} A_L \right]^{-1} \left[I - \frac{i\beta}{2} A_U \right] i\beta A \right\} k^n \\
&= R k^n ,
\end{aligned}
$$

where $\beta = (\Delta t \sin \omega \Delta x)/\Delta x$. If we let $\alpha = \beta u/2$, then the amplification matrix R is given by $R = I + 2\alpha F/(1+i\alpha)$ where the matrix F is given by

$$F = \begin{bmatrix} -i & -\dfrac{\alpha}{u^2} & -\dfrac{i\rho(1-i\alpha)}{u} \\ 0 & -(i+\dfrac{\alpha}{M^2}) & -\dfrac{i\rho u(1-i\alpha)}{M^2} \\ 0 & \dfrac{i(\alpha^2/M^2-1)}{\rho u(1+i\alpha)} & -\dfrac{\alpha}{M^2}\dfrac{(1-i\alpha)}{(1+i\alpha)} - i \end{bmatrix} .$$

Here M denotes the Mach number. If we denote the eigenvalues of F by μ_j $(j = 1, 2, 3)$, then the eigenvalues of R are $(1 + i\alpha + 2\alpha\mu_j)/(1 + i\alpha)$. Let $z_j = 1 + i\alpha + 2\alpha\mu_j$; then by expanding the characteristic equation of F to find an equation for μ_j we obtain $z_3 = 1 - i\alpha$, $(z_j + Q_1)(z_j + Q_2) = -Q_3$ $(j = 1, 2)$ where

$$Q_1 = \alpha i + \frac{2\alpha^2}{M} - 1 ,$$

$$Q_2 = \alpha i + \frac{2\alpha^2(1-i\alpha)}{M^2(1+i\alpha)} - 1 ,$$

$$Q_3 = \frac{4\alpha^2(1-\alpha^2/M^2)(1-i\alpha)}{M^2(1+i\alpha)} .$$

Then $z_1 + z_2 = -(Q_1 + Q_2) = (1 - i\alpha)(2 - 4\alpha^2/(M^2(1+\alpha^2)))$ and $z_1 z_2 = (1 - i\alpha)^2$. Let $z_j = a_j(1 - i\alpha)$, then $a_1 a_2 = 1$ and $a_1 + a_2 = 2 - 4\alpha^2/(M^2(1+\alpha^2))$. The eigenvalues of R are $r_3 = (1 - i\alpha)/(1 + i\alpha)$ and $r_j = z_j/(1 + i\alpha)$ $(j = 1, 2)$. Thus $|r_1| = 1$, and $|r_j| = |a_j|$ $(j = 1, 2)$. Therefore $|r_j| \leq 1$ $(j = 1, 2, 3)$ if and only if $\alpha^2 \leq M^2(1+\alpha^2)$. This follows from the product and sum relations for a_j. Therefore we have unconditional stability if $M \geq 1$. If $M < 1$, then the inequality $\alpha^2 \leq M^2(1+\alpha^2)$ reduces to $\beta^2 c^2 \leq 4 + \beta^2 u^2$ or $\Delta t \leq 2\Delta x/\sqrt{c^2 - u^2}$ where c is the velocity of sound. This completes the stability analysis.

We will now analyze the stability of the uncentered scheme defined by equations (2.2). Again we use the von Neumann method. The amplification matrix R is $R = C_1^{-1} C_2$ where $C_1 = I + \beta A_L$, $C_2 = I - \beta A_U$, and $\beta = i \Delta t \sin \omega \Delta x / \Delta x$. We first assume that $A(w)$ is constant, symmetric and positive definite. We can then prove that $\|R\| < 1$. The proof is almost exactly the same as that given by Ostrowski to prove that the Gauss-Sidel iterations converge [2]. Assume, for simplicity, that the order of A is three. Let $e_1 = (1, 0, 0)$, $e_2 = (0, 1, 0)$ and $e_3 = (0, 0, 1)$. Let x_o be an arbitrary three-dimensional vector, and let $[x]_i$ denote the i-th component of a vector x. Let $x_1 = x_o + \alpha_1 e_1$, $x_2 = x_1 + \alpha_2 e_2$ and $x_3 = x_2 + \alpha_3 e_3$ where α_i is chosen such that $[C_1 x_j]_j = [C_2 x_{j-1}]_j$ $(j = 1, 2, 3)$. It is easy to show that $C_1 x_3 = C_2 x_o$. We continue this process to obtain a sequence of vectors x_j such that $C_1 x_{3j} = C_2 x_{3j-3}$. We will show that $|x_j| \to 0$ (for $\beta \neq 0$) which can only occur if $\|C_1^{-1} C_2\| \leq 1$. Thus we will have proved stability. Since A is symmetric and positive definite we can define a norm for complex vectors x by $\|x\| = x^* Ax$. We have $x_{j+1} = x_j + \alpha_{j+1} e_k$ where $1 \leq k \leq 3$. A little algebra will yield

$$\|x_j\| - \|x_{j-1}\| = 2 \operatorname{Re} \left\{ \bar{\alpha}_j [Ax_{j-1}]_k \right\} + \bar{\alpha}_j \alpha_j a_{kk} .$$

From the definition of x_j we have $[C_1 x_{j+1} - C_2 x_j]_k = 0$. From this we have $[\beta A x_j]_k = \alpha_j (1 - \beta a_{kk})$. Therefore $\|x_{j+1}\| - \|x_j\| = -\alpha_j \bar{\alpha}_j a_{kk} < 0$. This in turn yields the convergence of $\|x_{j+1}\|$ which shows that $\alpha_j \to 0$. Since $[\beta A x_j]_k = \alpha_j (1 - \beta a_{kk})$ we can prove that $x_j \to 0$.

If the matrix A is given by equations (2.1) we are no longer able to obtain a stability condition by analytic means. However we can compute the eigenvalues of the amplification matrix numerically and thus determine a stability condition. The difference equation is

$$w^{n+1} = w^n - \Delta t \, A_L(w^n) \, w_{\hat{x}}^{n+1} - \Delta t \, A_U(w^n) \, w_{\hat{x}}^n .$$

If $A(w)$ is defined by equations (2.1), then the amplification matrix for this scheme is

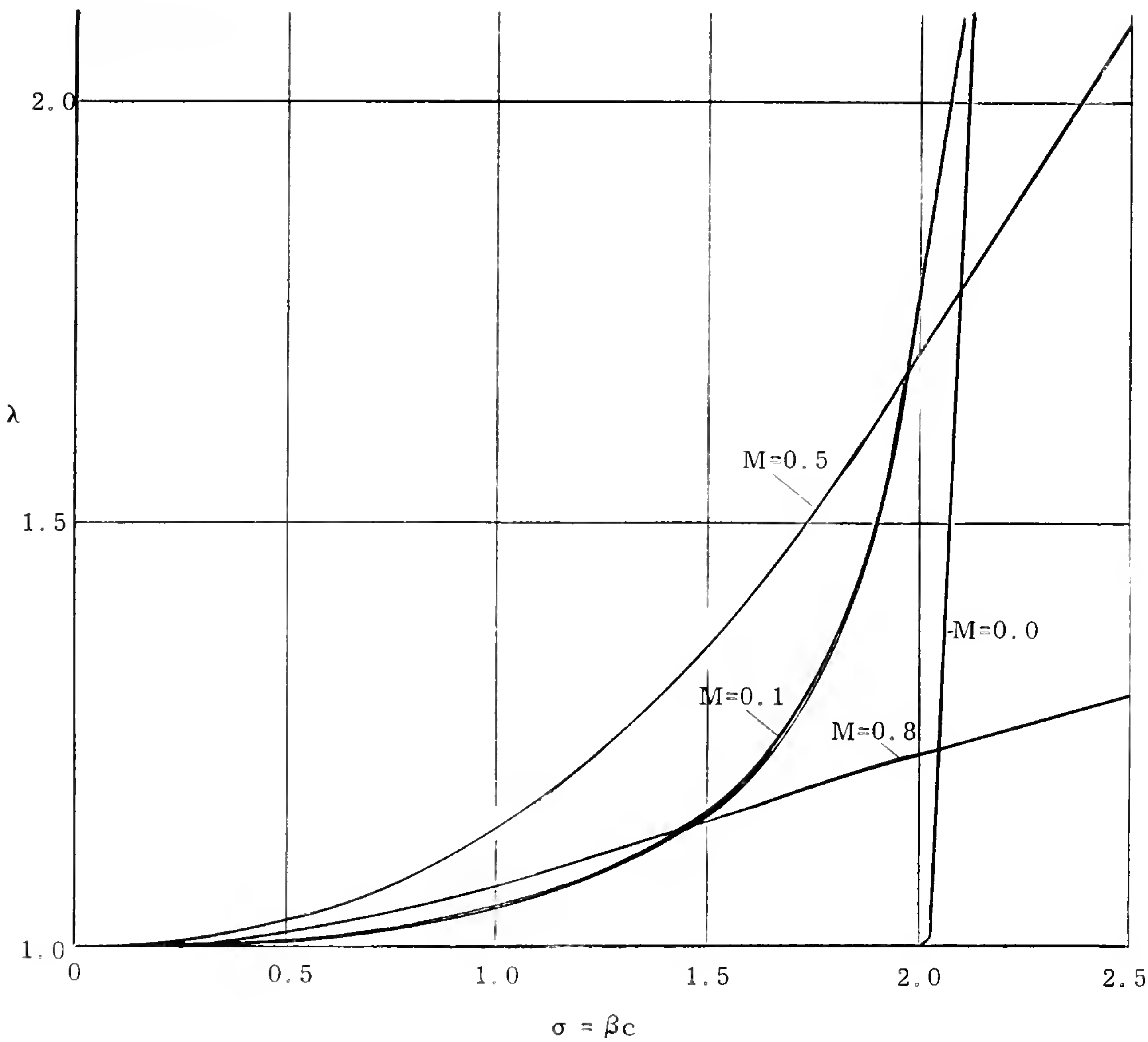

Figure 1. Stability of the Q-C-N scheme (uncentered)

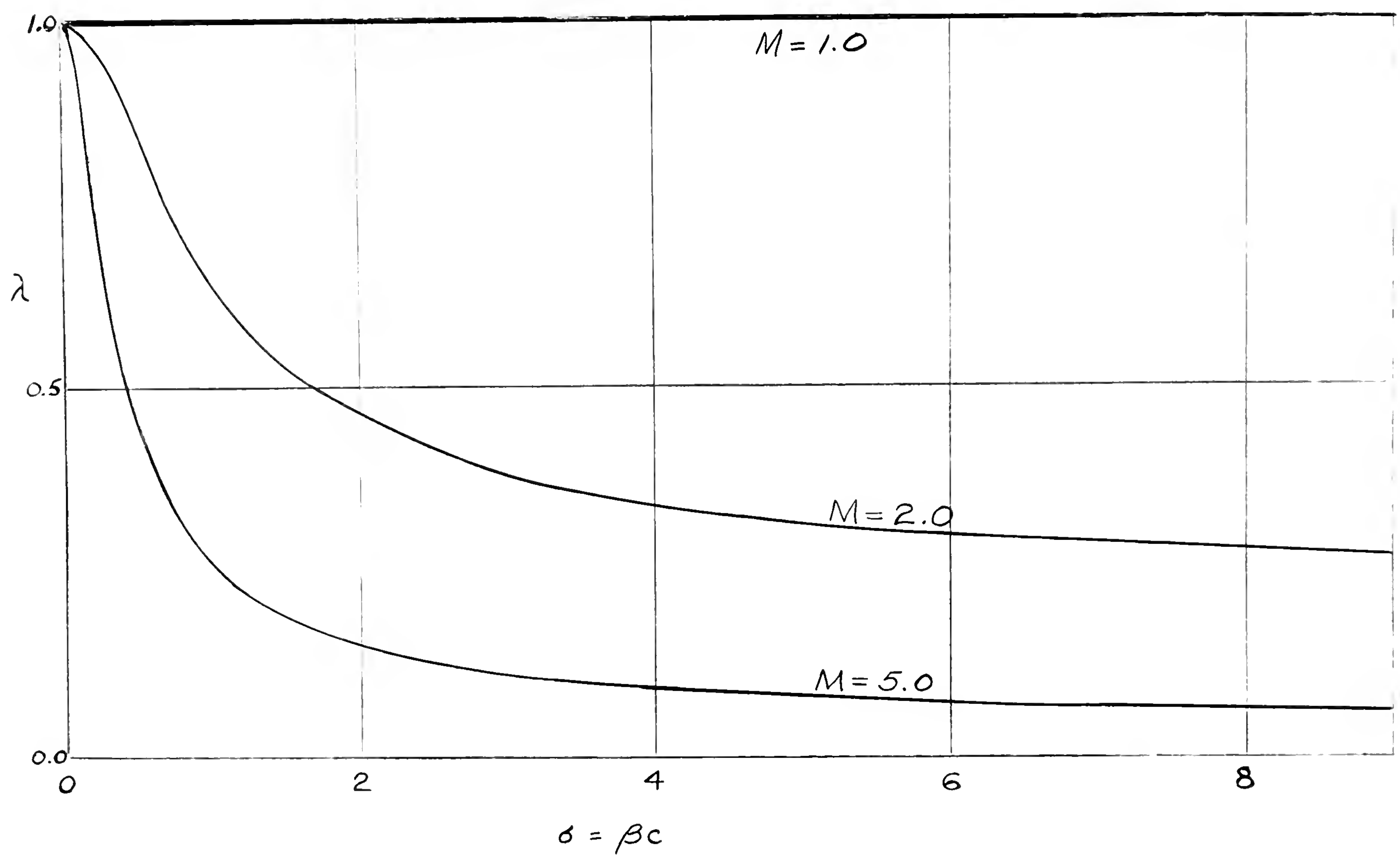

FIGURE 2. STABILITY OF THE Q-C-N SCHEME (UNCENTERED)

$$R = \begin{bmatrix} \frac{1}{1+i\alpha} & 0 & -\frac{i\beta\rho}{1+i\alpha} \\ 0 & \frac{1}{1+i\alpha} & -\frac{i\beta\gamma p}{1+i\alpha} \\ 0 & \frac{-i\beta}{\rho(1+i\alpha)^2} & \frac{-\beta^2\gamma p}{\rho(1+i\alpha)^2} + \frac{1}{1+i\alpha} \end{bmatrix} ,$$

where $\beta = (\Delta t \sin \omega \Delta x)/\Delta x$ and $\alpha = \beta u$. The eigenvalues of R are given by $\mu_j/(1+i\alpha)$ where $\mu_3 = 1$ and μ_j $(j = 1, 2)$ are the roots of the following quadratic

$$\mu^2 - (2-\delta)\mu + 1 = 0 \quad , \qquad \delta = \frac{\beta^2 c^2}{1+i\alpha} \quad .$$

Note that the eigenvalues of R depend only on $\sigma = \beta c$ and $M = u/c$. We let λ denote the absolute value of the largest eigenvalue of R. In Figures 1 and 2 λ is plotted against σ for various values of the Mach number M. These graphs indicate that the scheme is unconditionally stable for $M > 1$ and unconditionally unstable for $M < 1$. Numerical computations were performed using this scheme as described in Section 3. The flow was a rarefaction wave with $M = 2.0$ ahead and $M = 1.75$ behind the wave. If the value of Δt was made equal to ten times the value of Courant-Friedrichs-Lewy (i.e., $\Delta t = 10\,\Delta x/(|u|+c)$), then there was no sign of instability out to 44 time steps. Computations were also performed with a subsonic rarefaction wave with $M = 0.0$ ahead and $M = 0.7$ behind the wave. With $\Delta t = 2\,\Delta x/(|u|+c)$ the density became negative at 61 time steps and when $\Delta t = \Delta x/(|u|+c)$ the density was negative at 377 time steps. For small values of Δt the largest eigenvalue of the amplification matrix R is very close to the unit circle, therefore instability is slow to develop.

The eigenvalues of M drop off quite rapidly for supersonic flow according to Figure 2. This suggests that the scheme might produce reasonable results

even if the flow contains a shock. We tested this scheme on a flow which was initially an isentropic compression wave. Eventually the compression wave will produce a shock. This provides a test of how the difference scheme will react to the shock. We ran the Lax-Wendroff scheme on the same flow for a comparison. The initial compression wave had a Mach number of 2.53 behind and 1.5 ahead, which produced a very strong shock. The computed values of pressure are plotted in Figure 3. Both schemes were run to 300 time steps (at $\Delta x = 0.05$). By printing out the computed value of pressure every 40 time steps from 100 to 300 time steps and observing where the shock is located we can compute the shock velocity. For both schemes the shock velocity is constant within the accuracy of measurement. We know the state ahead of the shock; thus we can compute the state behind the shock from the shock velocity and the Rankine-Hugoniot relations. The results are given in the table below.

	Lax-Wendroff		Quasi-C.-N.	
	Observed	Computed from R-H	Observed	Computed from R-H
Shock Mach number	3.00	---	2.33	---
Pressure ratio	10.2	10.3	10.7	6.17
Density ratio	3.84	3.85	5.4	3.12
Velocity behind	3.70	3.72	3.65	3.11

When Δx is reduced to 0.02 the results from the quasi-C.N. scheme do not improve. The observed shock speed is 2.34 for $\Delta x = 0.02$. The computed value of pressure for $\Delta x = 0.02$ is plotted in Figure 3. This lack of improvement is to be expected since the state immediately behind the shock is nearly constant. Thus the results from the Q.-C.-N. scheme are apparently worthless, although the curves in Figure 3 appear reasonable upon casual inspection.

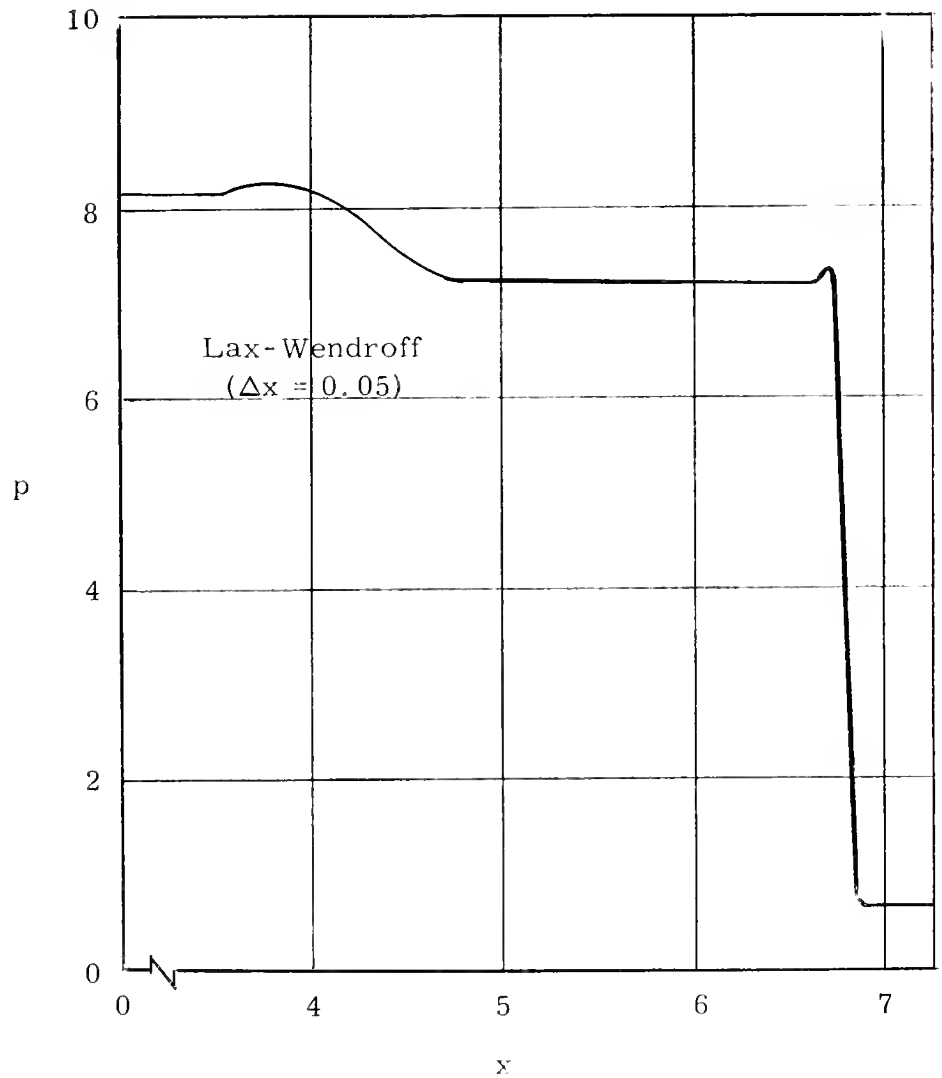

Figure 3. Pressure p vs. distance x at 150 time-steps

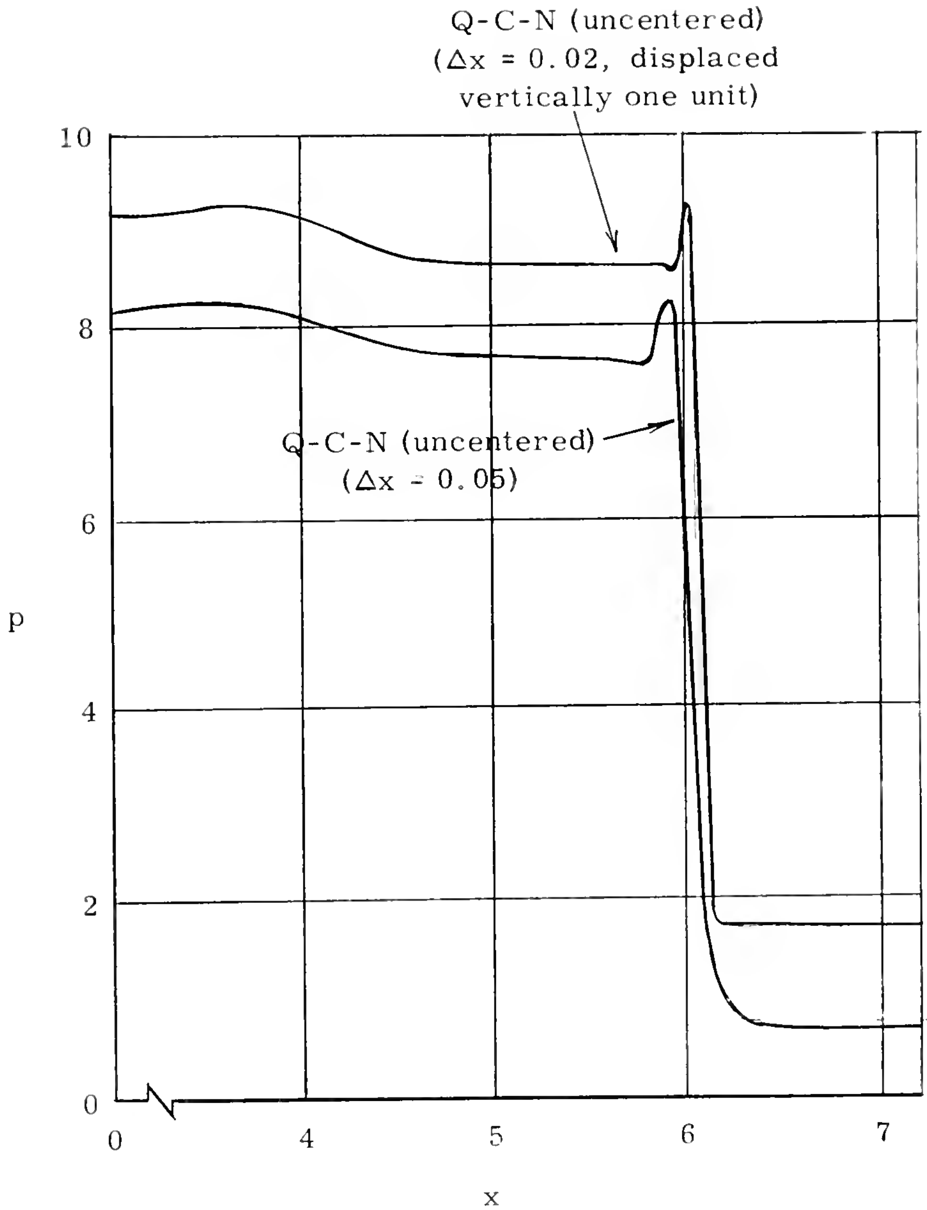

Figure 3 (Continued)

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